

The Dispersion of Cu Metallic Quantum Well States in Cu/Ni/Cu(100)

A. Danese,¹ R.A. Bartynski,¹ D.A. Arena,² M. Hochstrasser,² and J. Tobin²

¹Department of Physics and Laboratory for Surface Modification
Rutgers University, 136 Frelinghuysen Rd., Piscataway, NJ 08855

²Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory
Livermore, CA

It is well known that the magnetic coupling between successive ferromagnetic layers in multi-layer structures composed of alternating ferromagnetic/nonmagnetic (FM/NM) films oscillates between parallel and antiparallel as a function of the NM film thickness.[1,2] This oscillatory magnetic coupling gives rise to the giant magnetoresistance effect in these structures, a phenomenon that has been attributed to the formation of metallic quantum well (MQW) states in the NM layer.[3-10] In particular, with increasing NM film thickness, MQW states cross extremal points of the NM layer's Fermi surface (at the belly and the neck of the Fermi surface for Cu) with a periodicity identical to that of the oscillatory magnetic coupling.

Using a phase analysis approach, we have modeled the behavior of Cu MQW states in the Cu/fccNi(100), Cu/fccCo(100) and Cu/fccFe(100) systems.[5,9,10] The variation of MQW state energies with Cu film thickness and the states' dispersions with parallel momentum (k_{\parallel}) are well described by these calculations. We have found that the projected band gaps of the FM layer can influence the MQW states of the NM layer in two important ways. First, the thickness at which a given MQW state crosses the Fermi level depends on the energy at which the projected band gaps of the FM layer occur. In addition, the dispersion with k_{\parallel} of a Cu MQW state gets uncharacteristically flat (i.e. has a high effective mass) when the energy of the state falls in a projected band gap of the FM layer.

In earlier inverse photoemission (IPE) studies, [5,9,10] we have verified this latter situation for the Cu/fccCo/Cu(100) system. Since similar band gaps occur for fccNi and fccFe, MQW states in Cu films grown on those substrates should have flat MQW bands in the same region of k_{\parallel} . In Fig. 1, the projected band gaps of Fe, Co and Ni along the $\bar{\Gamma}\bar{X}$ direction of the film's two-dimensional Brillouin Zone (2DBZ) are plotted along with the projected band gaps of Cu. As one can see, the Co band gap near the neck of the Cu Fermi surface straddles the Fermi level. In contrast, the corresponding gap is centered about 1 eV above the Fermi energy (E_F) in fccFe(100), and about 1 eV below E_F in fccNi(100). This suggests several interesting possibilities. First, we expect that IPE measurements will reveal a flat Cu MQW band above the Fermi level in the Cu/fccFe/Cu(100) system and ARPES should show one below the Fermi level for Cu/fccNi/Cu(100). Furthermore, as these are minority spin gaps in the FM, these flat MQW bands should be spin polarized.

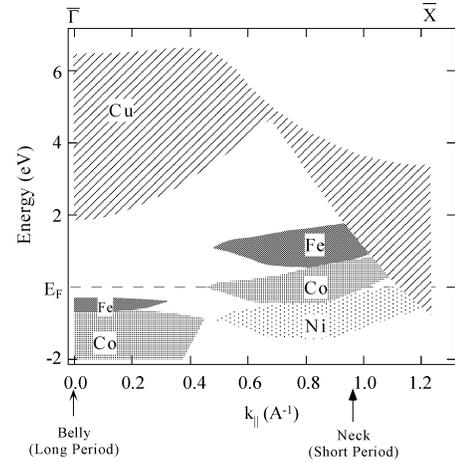


FIG. 1: (100) projected band gaps of Cu, fcc Fe, fccCo, and fccNi.

Using the UltraESCA end station of Beamline 7.0.1, we have obtained preliminary photoemission data from the Cu/fccNi/Cu(100). The sample was prepared by depositing ~ 35 ML of Ni onto an atomically clean, well-ordered Cu(100) surface. This was followed by deposition of a

wedge-shaped Cu film whose thickness ranged from 0 to 30 ML. Figure 2 show a series of normal emission photoemission data displayed as a 2-dimensional plot of Cu film thickness vs. binding energy. Light colors indicate high intensity and the dark colors low. As has been seen on other similar systems, we find a series of intensity maxima that move towards the Fermi level as the film thickness increases. These peaks are associated with metallic quantum well states in the Cu films whose energy changes with film thickness. The presence of these states confirms the quality of our films. The period with which these Cu MQW states cross E_F appears to be longer than has been observed for the Cu/fccCo system. This may indicate that the Ni layer is no longer pseudomorphic and has reverted back to its unstrained structure. As a result, the Cu overlayer may be tetragonally distorted with an increased spacing perpendicular to the plane of the film which gives rise to a smaller Fermi surface spanning vector and thus a larger thickness period. Quantitative structural studies and first principles electronic structure calculations are currently underway to investigate this effect.

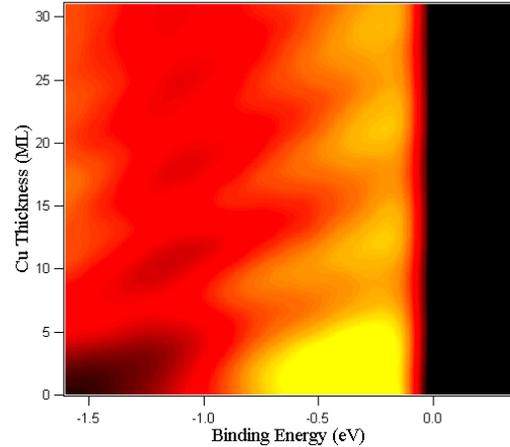


Fig. 2.: Normal emission from the Cu/Ni/Cu(100) system as a function of Cu film thickness.

Turning our attention to the MQW states away from the center of the 2DBZ, two important findings are summarized in Fig. 3. The left panel shows a series of photoemission spectra obtained for Cu thicknesses ranging from 5 to 14 ML near the X point of the 2DBZ. Even at this large value of $k_{||}$, the Cu MQW states are clearly visible. The right panel shows a spectrum obtained at $k_{||} = 0.75 \text{ \AA}^{-1}$ that exhibits two distinct features, a strong sharp peak near E_F , and a second broader peak at a binding energy of 0.85 eV. The higher binding energy feature occurs in exactly the region of energy and momentum where the projected band gap

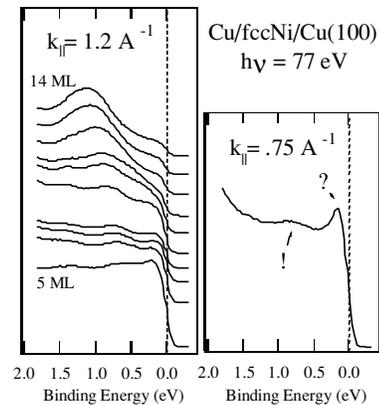
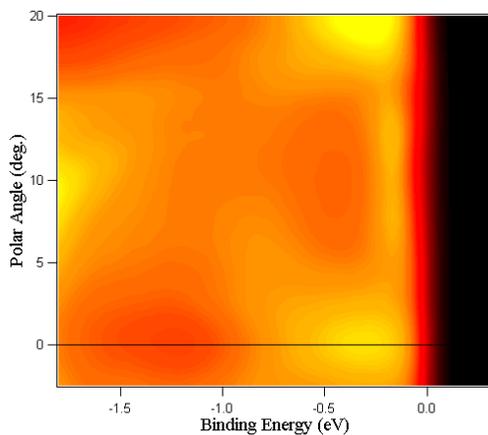
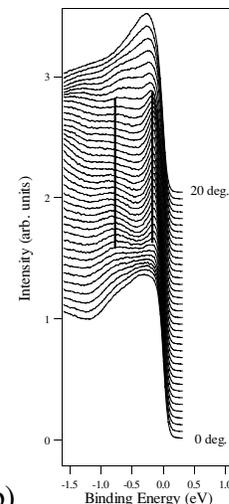


FIG. 3: Cu/fccNi/Cu(100) ARUPS spectra.



(a)



(b)

Fig. 4: Angular scan from the 7 ML Cu/Ni/Cu(100) system exhibiting two nondispersing MQW states.

of fccNi is predicted (*c.f.* Fig. 1) and is identified as a Cu MQW state. In contrast to the Cu/fccCo IPE data, however, this MQW feature is much weaker. Most likely the lower intensity is due to a smaller reflectivity at the Cu/Ni interface. The nature of the feature at the Fermi level is less obvious.

To investigate the dispersion with k_{\parallel} of these features, we obtained photoemission data for a wide range of angles along the ΓX direction of the 2DBZ. Figure 4(a) shows a 2-dimensional map of the data while Fig. 4(b) displays the spectra as a function of energy and angle in conventional form. The two straight lines in Fig. 4(b) illustrate how the two spectral features show essentially no dispersion. The sharp peak just below the Fermi edge is totally unexpected from our simple model calculations and it is not present in the Ni film. As seen in Fig. 4, this feature persists for a wide range of the surface Brillouin zone. Recent inverse photoemission measurements from the same system show a similar feature just above the Fermi level. This suggests that this feature actually straddles E_F . Both of these features are observed for a range of Cu and Ni thicknesses. First principles density functional calculations are also underway to investigate the nature of these states.

REFERENCES

- [1] P. Grunberg et al., Phys Rev. Lett. **57**, 2442 (1986).
- [2] S.S.P. Parkin, N. Moore, K.P. Roche, Phys. Rev. Lett. **64**, 2304 (1990).
- [3] J.E. Ortega and F.J. Himpsel, Phys. Rev. Lett. **69**, 844 (1992).
- [4] P. Segovia, E.G. Michel and J.E. Ortega, Phys. Rev. Lett. **77**, 2734 (1996).
- [5] F.G. Curti, A. Danese and R.A. Bartynski, Phys. Rev. Lett. **80**, 2213 (1998).
- [6] R.K. Kawakami et al., Phys. Rev. Lett. **80**, 1754 (1998).
- [7] R.K. Kawakami et al., Nature. **398**, 132 (1999)
- [8] R.K. Kawakami et al., Phys. Rev. Lett. **82**, 4098 (1999).
- [9] A. Danese and R.A. Bartynski, Phys. Rev. B. (submitted).
- [10] A. Danese, D.A. Arena and R.A. Bartynski, Prog. Surf. Sci. (in press).

This work is supported by NSF Grant DMR-98-01681 and Petroleum Research Fund Grant # 33750-AC5,6.

Principle Investigator: Robert A. Bartynski, Department of Physics and Laboratory for Surface Modification, Rutgers University. Email: bart@physics.rutgers.edu. Telephone: 732-445-4839